The Method of Maximum Likelihood

James R. Graham

2014/9/21

Maximum Likelihood

Experiments select a sample from the parent population

- Suppose we select N points from a Gaussian parent distribution, with mean μ and standard deviation, σ
- The probability of making any single observation, x_i, is

$$P_i = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{x_i - \mu}{\sigma} \right)^2 \right]$$

Maximum Likelihood

We do not know μ or σ *a priori*

– μ must be derived from the data

– Denote this estimate μ'

What expression for μ' gives the ***maximum likelihood*** that the parent population has a particular mean given a set of data?

Using Maximum Likelihood to estimate the mean

Suppose the parent population has a mean μ' and a known standard deviation σ

– The probability of observing the i-th point x_i is

$$P_i\left(x_i \mid \mu'\right) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x_i - \mu'}{\sigma}\right)^2\right]$$

Estimating μ

Consider all N observations

– If the measurements are independent the probability for observing that set is the product of the individual $P_i(\mu')$

$$P\left(\left\{x_1, x_2, \ldots x_N\right\} \mid \mu'\right) = \prod_{i=1}^{N} P_i\left(x_i \mid \mu'\right)$$

$$= \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \exp\left[-\tfrac{1}{2}\sum_{i=1}^{N}\left(\frac{x_i - \mu'}{\sigma}\right)^2\right]$$

Estimating μ

According to the method of ***maximum likelihood*** we should compare the $P(\mu')$ for various parent populations with different μ' (all with the same σ)

- The probability is greatest that the data were derived from a population with $\mu' = \mu$
- We assert that the ***most likely*** parent population is the correct one

We are assuming, using Bayes' theorem

$$P\left(\mu' \mid \left\{x_1, x_2, \ldots x_N\right\}\right) = P\left(\left\{x_1, x_2, \ldots x_N\right\} \mid \mu'\right)$$

Calculating the mean

- According to maximum likelihood the most probable value of μ' is the one which gives the maximum probability, $P(\mu')$
  - Maximize

$$P(\mu') = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \exp\left[-\frac{1}{2}\sum\left(\frac{x_i-\mu'}{\sigma}\right)^2\right]$$

$$\propto \exp\left[-\chi^2/2\right]$$

or minimize, χ^2

$$\chi^2 = \sum\left(\frac{x_i-\mu'}{\sigma}\right)^2$$

Calculating the mean

- Find the minimum of χ^2 from the derivative

$$\frac{\partial \chi^2}{\partial \mu'} = \frac{\partial}{\partial \mu'} \sum \left(\frac{x_i - \mu'}{\sigma} \right)^2 = 0$$

$$= \sum \frac{\partial}{\partial \mu'} \left(\frac{x_i - \mu'}{\sigma} \right)^2 = 2 \sum \frac{x_i - \mu'}{\sigma^2} = 0$$

since the derivative of a sum is the sum of the derivatives

Calculating the mean

- The most probable value for the mean is given by

$$\sum \left(x_i - \mu' \right) = 0$$

$$\sum x_i - \sum \mu' = 0$$

$$\boxed{\mu' = \frac{1}{N} \sum x_i}$$

Weighting data

Suppose some measurements are better than others, some values are drawn from a population with smaller σ_i

– Maximize

$$P(\mu') = \prod_{i=1}^{N} \left(\frac{1}{\sigma_i \sqrt{2\pi}} \right) \exp\left[-\frac{1}{2} \sum \left(\frac{x_i - \mu'}{\sigma_i} \right)^2 \right]$$

Weighted mean

Maximizing the probability is equivalent to minimizing the argument in the exponential

$$\frac{\partial}{\partial \mu'} \sum \left(\frac{x_i - \mu'}{\sigma_i} \right)^2 = 2 \sum \frac{x_i - \mu'}{\sigma_i^2} = 0$$

$$\boxed{\mu' = \frac{\sum w_i x_i}{\sum w_i}, \quad w_i = 1/\sigma_i^2}$$

The most probable value of the mean is the ***weighted*** (inversely by the variance) mean

Error in the weighted mean

If $y = f(x_1, x_2, x_3\ldots)$ The fundamental law of error propagation is

$$\sigma_y^2 = \left(\frac{\partial f}{\partial x_1}\right)^2 \sigma_{x_1}^2 + \left(\frac{\partial f}{\partial x_2}\right)^2 \sigma_{x_2}^2 + \left(\frac{\partial f}{\partial x_3}\right)^2 \sigma_{x_3}^2 + \ldots$$

For a quantity where the errors in $x_1, x_2\ldots$ are uncorrelated

Error in the weighted mean

If we apply this to the formula for σ'

$$\sigma_{\mu'}^2 = \left(\frac{\partial \mu'}{\partial x_1}\right)^2 \sigma_1^2 + \left(\frac{\partial \mu'}{\partial x_2}\right)^2 \sigma_3^2 + \left(\frac{\partial \mu'}{\partial x_3}\right)^2 \sigma_3^2 + \ldots$$

$$= \sum_j \left(\frac{\partial \mu'}{\partial x_j}\right)^2 \sigma_j^2$$

Error in the weighted mean

So the tricky part is computing

$$\frac{\partial \mu'}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\sum_i w_i x_i}{\sum_i w_i}\right)$$

Working out the derivative

$$\frac{\partial \mu'}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\sum_i w_i x_i}{\sum_i w_i}\right)$$

$$= \left(\sum_i w_i\right)^{-1} \sum_i \frac{\partial}{\partial x_j}\left(w_i x_i\right)$$

$$= \left(\sum_i w_i\right)^{-1} \sum_i w_i \delta_{ij}$$

$$= \left(\sum_i w_i\right)^{-1} w_j$$

Putting it all together

$$\sigma_{\mu'}^2 = \sum_j \left(\frac{\partial \mu'}{\partial x_j} \right)^2 \sigma_j^2$$

$$= \sum_j \left(\frac{w_j}{\sum_i w_i} \right)^2 \sigma_j^2$$

$$= \left(\sum_i w_i \right)^{-2} \sum_j \left(w_j \sigma_j \right)^2, \qquad \text{but} \quad w_j = 1/\sigma_j^2$$

$$= \left(\sum_i w_i \right)^{-2} \sum_j w_j$$

$$= \left(\sum_i w_i \right)^{-1}$$

Error in the weighted mean

Or

$$\sigma_{\mu'}^2 = \left(\sum_i w_i \right)^{-1}$$

implies

$$\frac{1}{\sigma_{\mu'}^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2} + \cdots + \frac{1}{\sigma_N^2}$$

How to Fit a Straight Line

Suppose our data, y_i, are drawn from a population such that

$$y(x) = a_0 + b_0 x$$

For any x_i we can calculate the probability of making the observation y_i as

$$P_i = \frac{1}{\sigma_i \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left\{ \frac{y_i - y(x_i)}{\sigma_i} \right\}^2 \right]$$

Straight Line Fit

- The probability for making the observed set of measurements is the product

$$P\left(a_0,b_0\right)=\prod_{i=1}^{N}P_i$$

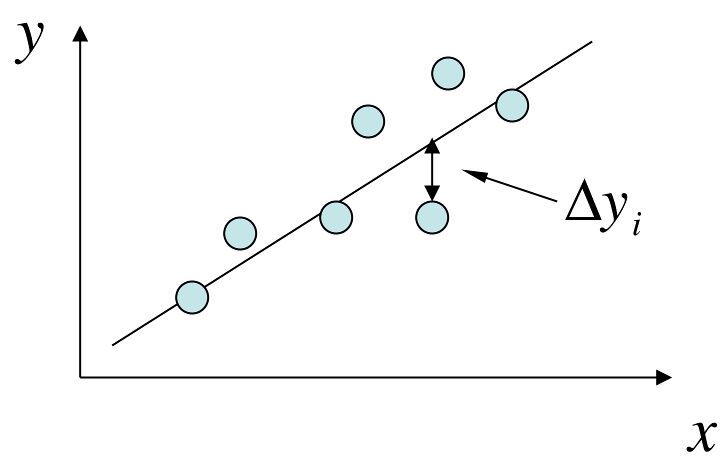
$$=\prod\left(\frac{1}{\sigma_i\sqrt{2\pi}}\right)\exp\left[-\tfrac{1}{2}\sum\left(\frac{y_i-y(x_i)}{\sigma_i}\right)^2\right]$$

Straight Line Fit

- Similarly, the probability for making the observed set of measurements given coefficients, *a* and *b* is

$$P(a,b) = \prod \left(\frac{1}{\sigma_i \sqrt{2\pi}} \right) \exp\left[-\tfrac{1}{2} \sum \left(\frac{\Delta y_i}{\sigma_i} \right)^2 \right]$$

$$\Delta y_i = y_i - a - b x_i$$



Straight Line Fit

- The product term is a constant, independent of a and b
  - Maximizing $P(a, b)$ is equivalent to minimizing the sum of the exponential

$$\chi^2 \equiv \sum \left(\frac{\Delta y_i}{\sigma_i} \right)^2$$

$$= \sum \frac{1}{\sigma_i^2} \left(y_i - a - bx_i \right)^2$$

Minimizing χ^2

- To find *a* and *b* which corresponds to the minimum χ^2 for constant σ

$$\frac{\partial}{\partial a}\chi^2 = \frac{\partial}{\partial a}\left[\frac{1}{\sigma^2}\sum\left(y_i - a - bx_i\right)^2\right]$$

$$= -\frac{2}{\sigma^2}\sum\left(y_i - a - bx_i\right) = 0$$

$$\frac{\partial}{\partial b}\chi^2 = \frac{\partial}{\partial b}\left[\frac{1}{\sigma^2}\sum\left(y_i - a - bx_i\right)^2\right]$$

$$= -\frac{2}{\sigma^2}\sum x_i\left(y_i - a - bx_i\right) = 0$$

Minimizing χ^2

- These can be rearranged to find pair of simultaneous equations for a and b which corresponds to the minimum χ^2

$$\sum y_i = aN + b\sum x_i$$

$$\sum x_i y_i = a\sum x_i + b\sum x_i^2$$

Minimizing χ^2

- Solving these of simultaneous equations

$$a = \frac{1}{\Delta}\begin{vmatrix} \sum y_i & \sum x_i \\ \sum x_i y_i & \sum x_i^2 \end{vmatrix}$$

$$b = \frac{1}{\Delta}\begin{vmatrix} N & \sum y_i \\ \sum x_i & \sum x_i y_i \end{vmatrix}$$

$$\Delta = \begin{vmatrix} N & \sum x_i \\ \sum x_i & \sum x_i^2 \end{vmatrix}$$

Example: Maximum Likelihood Estimators

- Suppose x_i is drawn from a Rayleigh distribution
  - e.g., distance of arrows from a bull's eye.

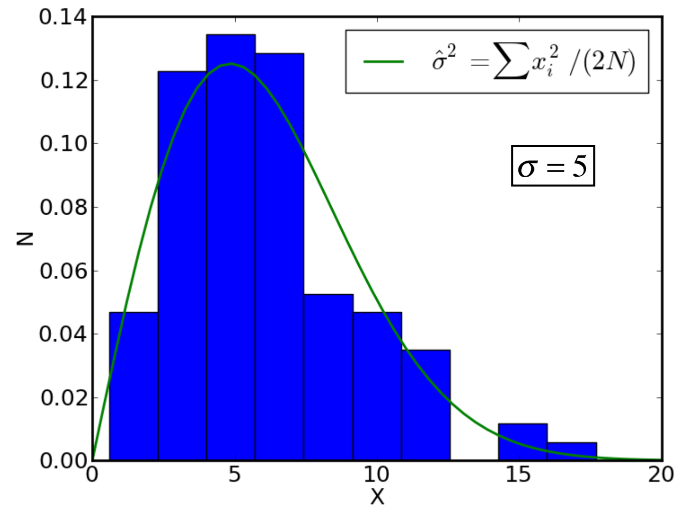
$$P(x) = \frac{x}{\sigma^2} \exp\left[-\frac{1}{2} \left(\frac{x}{\sigma} \right)^2 \right]$$

$$\langle x \rangle = \sqrt{\frac{\pi}{2}} \sigma, \quad \langle x^2 \rangle = 2\sigma^2, \quad \langle \sigma^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \frac{4-\pi}{2} \sigma^2$$

$$\log L = \log \prod_i \frac{x_i}{\sigma^2} \exp\left[-\frac{1}{2} \left(\frac{x_i}{\sigma} \right)^2 \right]$$

$$= \sum_i \left\{ \log\left[\frac{x_i}{\sigma^2} \right] - \frac{1}{2} \left(\frac{x_i}{\sigma} \right)^2 \right\}$$

$$\frac{\partial \log L}{\partial \sigma} = \sum_i \left\{ -\frac{2}{\sigma} + \frac{x_i^2}{\sigma^3} \right\} = 0; \quad -\frac{2N}{\sigma} + \frac{1}{\sigma^3} \sum_i x_i^2 = 0$$



The maximum likelihood estimator is $\hat{\sigma}^2 = \frac{1}{2N} \sum_i x_i^2$